The nonlinear conjugate gradient method is an iterative method using the conjugacy property of the matrix to solve a nonlinear system of equations. Details of the method can be found in *Numerical Optimization*(Nocedal, J., & Wright, S. (2006). Numerical optimization. Springer Science & Business Media.).

[called by: solvers.] [calls: packdof.]

Basic algorithm

The basic nonlinear conjugate gradient algorithm used in FOCUS is a hybrid of **Algorithm 5.4** and **Equation (5.49)** from *Numerical Optimization* and Dai & Yuan. This version of conjugate gradient method converges globally, provided the line search satisfies the standard Wolfe conditions.

Our target function is $\chi^2(\mathbf{X})$, while \mathbf{X} is the variables vector. As we mentioned before, we can calculate the gradient $G(\mathbf{X}) = \frac{\partial \chi^2}{\partial \mathbf{X}}$ accurately with analytical expressions. The structure of the algorithm is as below.

```
k=0: for initial \mathbf{X}_0, evaluate \chi^2(\mathbf{X}_0) and G(\mathbf{X}_0); p_0=-G_0; while G_k>\epsilon:
\mathbf{X}_{k+1}=\mathbf{X}_k+\alpha_k p_k \ (\alpha_k \text{ satisfies strong Wolfe condition});
\beta_{k+1}=\frac{|G_{k+1}|^2}{(G_{k+1}-G_k)^T p_k};
p_{k+1}=-G_{k+1}+\beta_{k+1} p_k ;
k=k+1 ;
end(while)
```

The line search algorithm is applying the **Algorithm 3.5 & 3.6** in the book to satisfy the strong Wolfe conditions.

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Focus subroutines;